

Product Name: GSK 3787

Catalog No.: 3961

Batch No.: 3

CAS Number: 188591-46-0

IUPAC Name: 4-Chloro-N-[2-[[5-(trifluoromethyl)-2-pyridinyl]sulfonyl]ethyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₂ClF₃N₂O₃S

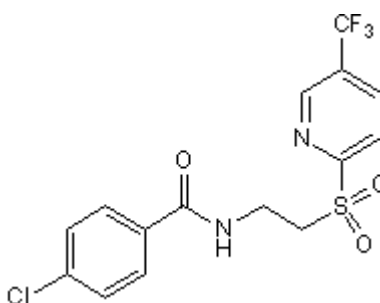
Batch Molecular Weight: 392.78

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.64 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	45.87	3.08	7.13
Found	45.84	3.2	7.11

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent and selective peroxisome proliferator-activated receptor δ (PPAR δ) antagonist (pIC_{50} = 6.6). Displays no measurable affinity for PPAR α or PPAR γ in vitro (pIC_{50} < 5).

Physical and Chemical Properties:

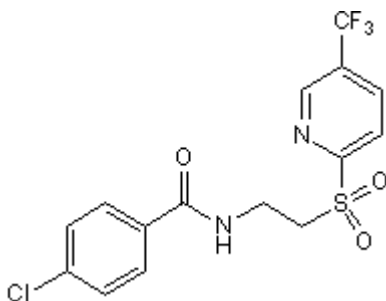
Batch Molecular Formula: C₁₅H₁₂ClF₃N₂O₃S

Batch Molecular Weight: 392.78

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Shearer et al (2010) Identification and characterization of 4-chloro-N-(2-[[5-(trifluoromethyl)-2-pyridinyl]sulfonyl]ethyl)benzamide (GSK3787), a selective and irreversible peroxisome proliferator-activated receptor delta (PPARdelta) antagonist. *J.Med.Chem.* **53** 1857. PMID: 20128594.

Palkar et al (2010) Cellular and pharmacological selectivity of the peroxisome proliferator-activated receptor- β/δ antagonist GSK3787. *Mol.Pharmacol.* **78** 419. PMID: 20516370.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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